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School of Life Sciences and Technology
School of Pharmacy
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ICMNS

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Science for Better Living

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Preface

ICMNS was held in ITB Campus, Bandung, 29 – 30 November 2006, under the joint auspices of Faculty of Mathematics and Natural Sciences, School of Pharmacy, and School of Life Sciences and Technology, Institut Teknologi Bandung.

We have been, almost, overwhelmed by the level of interest and participation in the conference. Overall, 13 invited lectures were delivered and 526 papers were presented (212 oral presentations and 314 poster presentations). The proceedings published in a CD-ROM form.

Space is unfortunately too short to thank individually all those people whose dedicated efforts, often over a period of many months, were responsible for the success of the conference - especially the members of the Steering and Organizing Committees.

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Robust Principal Component Analysis Using Minimum Covariance Determinant Estimator

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Abstract

Principal component analysis (PCA) is one of the most widely used statistical techniques for data dimension reduction. And a robust technique on PCA when data contains outlier is an important problem. In this paper, we consider the problem of robust PCA based on Minimum Covariance Determinant (MCD) mean and covariance matrix estimator. We aimed to look at the behavior of the principal component scores of robust PCA using MCD through their graphical plot of the first and the second PCS. The effect of outliers on PCA is studied by comparing the mean square error (MSE) resulted by MCD and by classical method in presence of outliers.

Keywords : *Robust, principal component analysis, minimum covariance determinant*

I. Introduction

Principal component analysis (PCA) is a popular statistical method which tries to explain the covariance structure of data by means of a small number of components. The main use of PCA is to reduce the dimensionality of a data set while retaining as much information as is possible. In essence, PCA seeks to reduce the dimension of the data by finding a few orthogonal linear combinations (the PCs) of the original variables with the largest variance. The first PC is the linear combination with the largest variance, the second PC is the linear combination with the second largest variance and orthogonal to the first PC, and so on. There can be as many possible PCs as there are variables.

Computation of PCs is based on a decomposition of covariance matrices. Let $\boldsymbol{x}$ be a p-dimensional random vector with $E(\boldsymbol{x}) = \boldsymbol{\mu}$ and $\mathrm{Cov}(\boldsymbol{x}) = \boldsymbol{\Sigma}$. The covariance matrix can be decomposed as $\boldsymbol{\Sigma} = \boldsymbol{\Gamma\Lambda\Gamma}^{\mathbf{T}}$, where the columns of $\boldsymbol{\Gamma} = (\boldsymbol{\gamma}_1, \boldsymbol{\gamma}_2, \ldots, \boldsymbol{\gamma}_p)$ are the eigenvectors of $\boldsymbol{\Sigma}$ and $\boldsymbol{\Lambda}$ is a diagonal matrix with the corresponding eigenvalues (arranged in descending order) of $\boldsymbol{\Sigma}$. The principal components of $\boldsymbol{x}$ are defined by $\boldsymbol{\xi} = \boldsymbol{\Gamma}^{\mathbf{T}}\boldsymbol{(x-\mu)}$. Classically, $\boldsymbol{\mu}$ is estimated by the sample mean $\bar{\boldsymbol{x}}$, and $\boldsymbol{\Sigma}$ by the sample covariance matrix $\boldsymbol{S}$, which is decomposed into eigenvectors and eigenvalues. $\bar{\boldsymbol{x}}$ as well as $\boldsymbol{S}$ are highly sensitive with respect to outlying observations. Therefore, data reduction based on classical PCA becomes unreliable if outliers are present in the data. A robust version of principal component analysis is needed.

There is a rich literature related to study of robust PCA, e.g 1) -2) -3) -4) -5 -6)). PCA can easily be robustified by estimating the multivariate scatter matrix $\boldsymbol{\Sigma}$ in a robust way. Many robust estimators of multivariate location and scatter have been investigated in the literature, such as M-estimators 7), the minimum volume ellipsoid and minimum covariance determinant estimator 8) and S-estimators 11). In this paper we use the minimum covariance determinant (MCD) estimator. The robustly estimated covariance matrix is not influenced by outliers, and hence the eigenvector/eigenvalue decomposition is also robust. Since the MCD additionally gives a robust estimation of $\boldsymbol{\mu}$, the whole PCA procedure is robust.

II. The MCD Method

Minimum covariance determinant estimator was first proposed by Rousseeuw 12). The estimator is defined as the mean and the covariance matrix of the halfset H containing h observations whose covariance matrix has the smallest determinant. The usual value of h, i.e. the one which achieves the highest breakdown point is $h = (n + p + 1)/2$, where n is the sample size and p is the number of variables. Since in general we cannot consider all h-subsets, we must rely on approximate algorithms. Rousseeuw and Van Driessen (1999) proposed a hybrid algorithm which they called the FAST-MCD. The algorithm can be described as follows:

1. Start with a fixed number, (K), of random elemental subsets and use them to construct corresponding halfsets.
2. Carry out two concentration steps (C-step) on the K halfsets and select a small number of "best" ones.
3. For the "best" halfsets, carry out C-steps until convergence and the FAST-MCD estimators are based on the halfset with the lowest determinant of the covariance matrix.

Basically a C-step consists of computing first the classical center $\hat{\mu}_0$ and the classical covariance matrix $\hat{\Sigma}_0$ of the *h* observations. Then the robust distance of each point is computed as :

$$RD\hat{}(\boldsymbol{x_i}) = \sqrt{(\boldsymbol{x_i} - \hat{\mu}_0)^t \hat{\Sigma}_0^{-1} (\boldsymbol{x_i} - \hat{\mu}_0)}$$

A new *h*-subset is formed by the *h* observations with smallest robust distance.

III. Simulation

To look at the performance of the principal component score based on classical and robust methods, we have generated p=5 dimensional data from a multivariate normal distribution $N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$. We considered data without outliers (ε = 0%) as well as contaminated data (ε = 10%, 20%, 30%, 40%). We report the results of three sample sizes we set: *n* = 20, 30 and 100. And for computing the MSE we have generated 500 data sets for every sample size.

IV. Result

The presented figures show the plot of the first and the second principal component scores of the original (uncontaminated) data (black dot), and the contaminated data with the classical PCA (blue "K") and robust PCA using MCD (red "R") for data sets with *n*= 100.

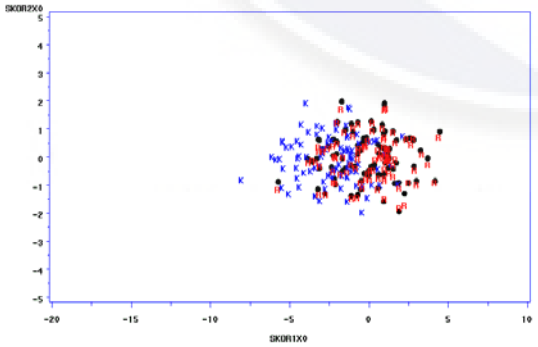

Figure 1. Plot of the first and the second PCS exclude outliers with n=100 and ε =10%

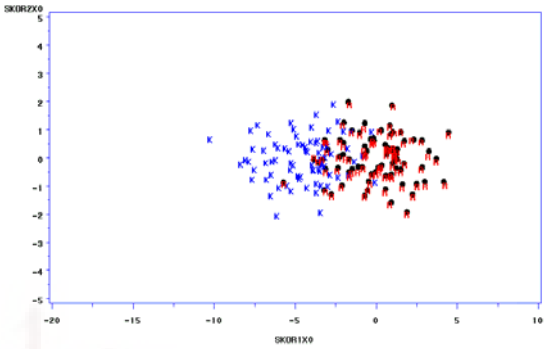

Figure 2. Plot of the first and the second PCS exclude outliers with n=100 and ε =20%

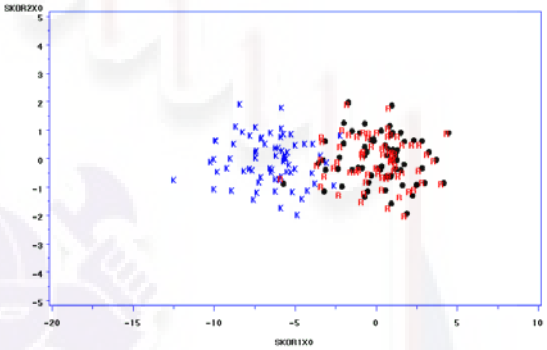

Figure 3. Plot of the first and the second PCS exclude outliers with n=100 and ε =30%

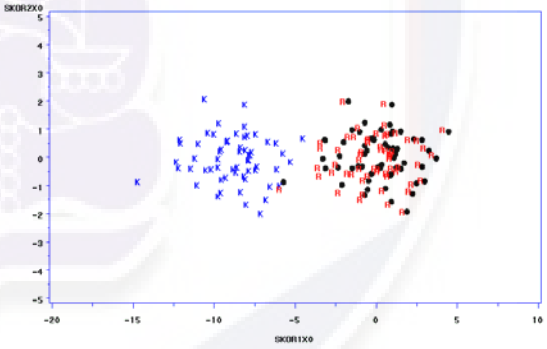

Figure 4. Plot of the first and the second PCS exclude outliers with n=100 and ε =40%

We see that the principal component scores of classical PCA are influenced by the outlier, the more outliers contained in the data the larger the deviation of classical principal component score from the original ones. While the principal component score resulted by MCD are very close to the original ones. The plot of the first and the second principal components scores (PCS) of data sets with *n*=20 and *n*=50 were similar to *n*=100 therefore not included, except for the case of *n*=20 and ε=40% the PCS of MCD changed very much, it is shown in Figure 5 below.

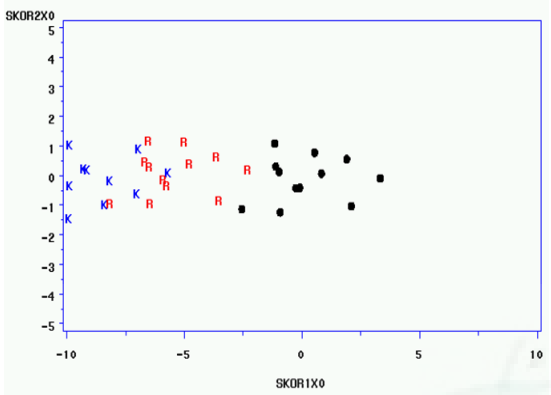

Figure 5. Plot of the first and the second PCS exclude outliers with n=20 and ε =40%

The mean square error (MSE) of the principal component scores was calculated over the 500 data sets:

$$\boldsymbol{MSE}(\hat{\xi}_i) = \frac{1}{500}\sum_{s=0}^{500}(\hat{\xi}_i^j - \hat{\xi}_i^0)^2 \ , \quad i=1,\ldots, n$$

Where $\hat{\xi}_i^j$ is the principal component score of the i-th observation on the j-th data set, and $\hat{\xi}_i^0$ is the principal component score of the i-th observation on the original data set (the uncontaminated data). The average MSE of principal component scores was calculated without counting the MSE of outliers. The values of the average MSE are reported in Table 1, and presented as curves in Figure 6.

Table 1. The average MSE of principal component scores.

ε	n=20		n=50	
	classic	MCD	classic	MCD
0%	0.002473	0.079116	0.002449	0.031496
10%	5.001963	0.215406	4.996395	0.028838
20%	20.039037	0.046588	19.985864	0.042380
30%	44.949452	0.104376	44.898085	0.012440
40%	79.914660	76.853898	79.801517	0.019434

Table 1 (continued)

ε	n=100	
	classic	MCD
0%	0.002514	0.011257
10%	4.997921	0.012080
20%	19.999591	0.005401
30%	45.006627	0.057622
40%	79.099709	0.072635

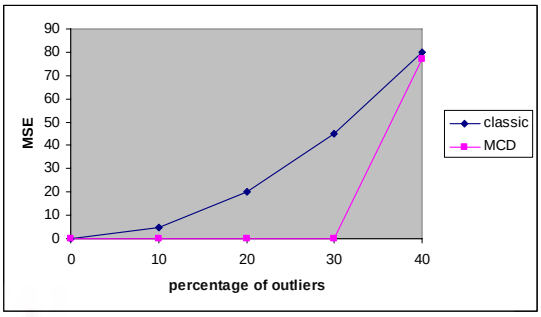

Figure 6 (a). The average MSE curve of classical and MCD principal component scores with n=20

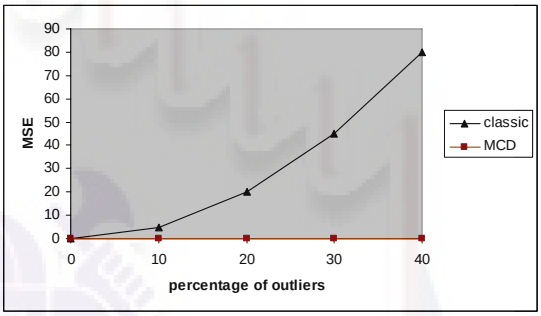

Figure 6 (b). The average MSE curve of classical and MCD principal component scores with n=50

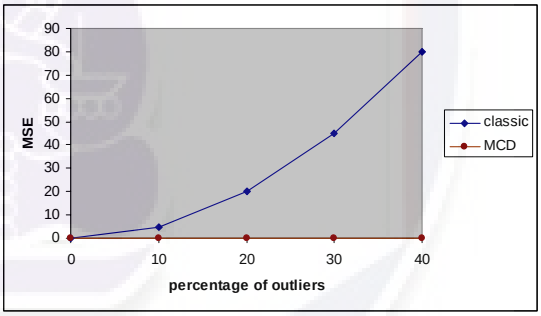

Figure 6 (c). The average MSE curve of classical and MCD principal component scores with n=100

Figure 6 gives the average MSE of principal component scores over 500 data set for different sample sizes. We see that the average MSE of principal component scores resulted by classical PCA is quadratic in ε, while the average MSE of principal component scores resulted by MCD is constant (except for n=20 and ε=40%) which means that the PCS of MCD is robust.

K

‘z

X’zx’a

V. Conclusion

In this paper we have shown the effect of outlier on principal component scores resulted by classical PCA and robust PCA using MCD. The MCD method performs much better than the classical method. Hence, robust PCA based on the minimum covariance determinant estimator is a good choice for PCA when data contains outliers and can easily be computed using statistical software packages, e.g. S-Plus or SAS.

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